ENERGY OF BINDING OF WATER AND ETHYL ALCOHOL WITH ACTIVE MOLECULAR OXYGEN FORMED AS A RESULT OF CONTACT OF A LIQUID WITH COARSELY DISPERSED NATURAL MINERAL FLINT

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Based on nuclear-magnetic resonance spectroscopic and diffractometric studies, a method is developed to calculate the energy of binding of water and ethyl alcohol with the molecular oxygen dissolved in liquids.

In [1], we have shown that in filtration of water through coarsely dispersed natural mineral flint clusters of the type $O_2^-.(H_2O)_n$ are formed in the water that become the nuclei of formation of a new structure of water. This modified structure of water is retained in different products.

The nature (mechanism) of formation of the cluster $O_2^-.(H_2O)_n$ reduces to transfer of an electron charge to a molecule of the oxygen dissolved in a liquid. To gain insight into this mechanism, it is necessary to determine the energy of binding of a water molecule and an ethyl-alcohol molecule with molecular oxygen.

First, we calculate the energy of binding of an H_2O molecule, being in ordinary water, with an O_2 molecule. For this purpose we employ the approach used in determination of the energy of hydrogen bonds in water [1]. As a calculational formula, we use the following relation:

$$E = \frac{2W_2^4}{|2W_3|^3} \sum_{\alpha > \beta} \cos^2 \theta_{\alpha\beta} \,, \tag{1}$$

$$W_2 = \eta_{ij\alpha} \frac{\hbar^2}{md^2} \,, \tag{2}$$

$$W_3 = \varepsilon_s^c - \varepsilon_p^a \,, \tag{3}$$

where d is the distance between nuclei, m is the electron mass, $\eta_{ij\alpha}$ is the parameter acquiring four universal constant values corresponding to matrix elements of the type $ss\sigma$, $sp\sigma$, $pp\sigma$, and $pp\pi$ (s, p, σ, and π are the symbols for the orbitals in an atom), and $\theta_{\alpha\beta}$ are the angles between the vectors formed by the central ions and the neighboring atoms.

In our work, consideration is given to the systems for which

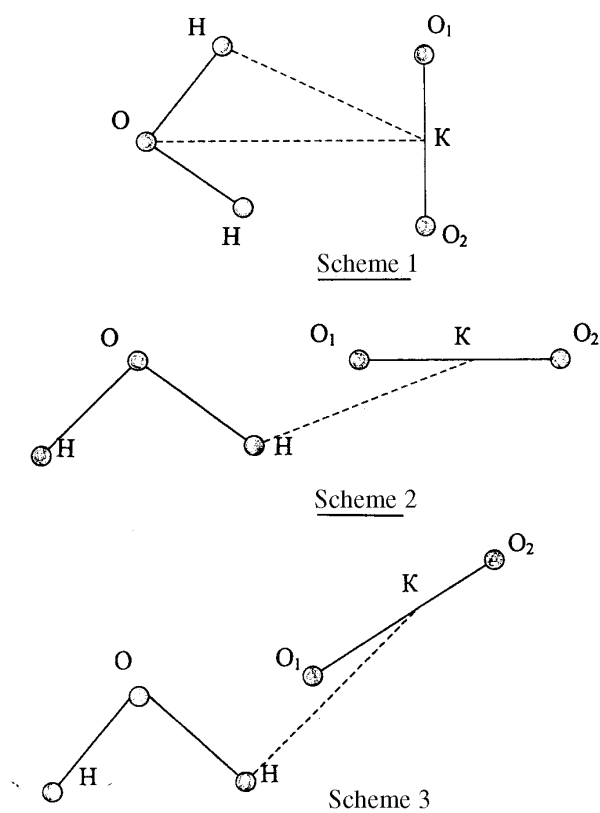$$\sum_{\alpha > \beta} \cos^2 \theta_{\alpha\beta} = 1 \,.$$

Fig. 1. Schemes of the interaction of a water molecule with molecular oxygen.

To perform the calculations, it is necessary to evaluate the term (electron energy level) of the oxygen atom in an O_2 molecule. According to [2], the hydrogen bond between a water molecule and a molecular oxygen molecule is formed due to interaction of the orbital $1s$ of the hydrogen atom in the H_2O molecule and of the antibonding orbital $3\sigma_u$ of the O_2 molecule. The term of the orbital $3\sigma_u$ is 20.106 eV.

As follows from [3], in its binding properties the molecular orbital $3\sigma_u$ is close to the orbital $2p\sigma$; however, it contains a noticeable contribution of the atomic orbital $2s$. Using the already known method [1], we find the term of electrons of the p-state of the orbital $3\sigma_u$. This term turns out to be equal to 15.894 eV. In the formula from [1], as the quantity d the distance between the hydrogen atom of a water molecule and the center of an oxygen molecule must be introduced, determined according to scheme 1 presented in Fig. 1. Such a configuration of $O_2^-.(H_2O)_n$ corresponds, according to [4], to interaction of an H_2O molecule with an O_2 molecule for the valence angles in H_2O that are larger than 98°.

When the length of the hydrogen bond is 1.825 $\overset{\circ}{A}$, d is equal to 1.922 $\overset{\circ}{A}$. In formula (1), as the dimensionless coefficient $\eta_{ij\alpha}$, the coefficient $\eta_{ss\sigma}$ for the cubic structure equal to 1.23 is adopted; then the energy of interaction is 0.0345 eV.

Now we pass to determination of the energy of interaction of a water molecule with a negative ion of molecular oxygen O_2^-. According to [5], the formation of the molecular ion O_2^- is related to spin splitting of the molecular orbital $3\sigma_u$ of oxygen.

In [6], it is noted that the state of the negative ion O_2^- emerges when to the core of O_2^+, being in the $a^4\pi_u$-state, two Rydberg electrons are added on the orbital $3G_g$.

The term of the orbital $3G_g$ in the O_2 molecule is 15.13 eV [2] and, as in the case of the orbital $3\sigma_u$, the term of electrons of the p-state of the orbital $3G_g$ in O_2 is 11.9636 eV. The question arises: "what value will the term of electrons of the p-state of the orbital $3G_g$ in an isolated ion O_2^- have and how does this

term change when O_2^- is in a liquid and is surrounded by a great amount of molecules of water and ethyl alcohol?"

For the isolated state of O_2^-, the term can be calculated as follows:

$$T_{3G_g[O_2^-]} = T_{3G_g[O_2]} \frac{D_{0[O_2^-]}}{D_{0[O_2]}}. \tag{4}$$

According to [7], $D_{0[O_2^-]} = 4.09$ eV. In [6], $D_{0[O_2]} = 5.08$ eV is reported. Then for the isolated ion O_2^- we have

$$T_{3G_g[O_2]} = 9.6314 \ \text{eV}.$$

The value of the term $T_{3G_g[O_2^-]}$ close to this quantity can be obtained if we construct the dependence

$$T_{3G_g[O_2^-]} = f\left[\frac{(r' - r'_e)}{r'_e}\right]. \tag{5}$$

According to the measurement data of the electron energy levels of O_2 given in [6], this dependence can be written in the following way:

$$T_{3G_g[O_2^-]} = T_{3G_g[O_2]} \exp\left[-1.795\left(\frac{r' - r'_e}{r'_e}\right)\right], \tag{6}$$

$r'_e = 1.205$ Å. For the isolated ion O_2^-, $r' = 1.341$ Å.

Using relation (6), we obtain

$$T_{3G_g[O_2^-]} = T_{3G_g[O_2]} \exp\left[-1.921\left(\frac{r' - r'_e}{r'_e}\right)\right]. \tag{7}$$

Taking the mean value of the multiplier in front of $\dfrac{r' - r'_e}{r'_e}$, we finally arrive at

$$T_{3G_g[O_2^-]} = T_{3G_g[O_2]} \exp\left[-1.858\left(\frac{r' - r'_e}{r'_e}\right)\right]. \tag{8}$$

Formula (8) makes it possible to calculate the term of electrons of the *p*-state of the orbital $3G_g$ for any intermediate configuration of the clusters $O_2^-.(H_2O)_n$ in liquids, but this requires knowledge of the quantity $\dfrac{r' - r'_e}{r'_e}$.

Evaluation of the parameter $\dfrac{r' - r'_e}{r'_e}$ in liquids from the data of experimental measurements is still impossible but it can be calculated. To do this, another approach must be employed.

As is mentioned in [1], the reason for formation of the negative ions of molecular oxygen in liquids is the transfer of a charge from the water molecules adsorbed on flint deep into the liquid along the chain of

hydrogen bonds (by the mechanism of proton conduction). The value of the charge is calculated from the estimates of deformations of the flint lattice.

In fact, the change in the distance between the nuclei in the oxygen molecule will be determined by the charge transfer. Then formula (8) can be written as

$$T_{3G_g[O_2^-]} = T_{3G_g[O_2]} \exp[-\beta \Delta q] . \tag{9}$$

For the cluster $O_2^-.(H_2O)_n$, according to [4] $\Delta q = 0.04$, consequently, $\beta = 5.243$.

It should be noted that the total energy of a biatomic molecule, of its molecular ion or the term of electrons of any orbital in the particular state is determined as

$$T = T_e + G_{(V)} + F_{V(J)} , \tag{10}$$

$$G_{(V)} = W_e (V + 0.5) - X_e \omega_e (V + 0.5)^2 , \tag{11}$$

$$F_{V(J)} = [B_e - a_e(V + 0.5)] J (J + 1) . \tag{12}$$

The parameters ω_e, $X_e\omega_e$, and a_e are presented in the tables of [6, 8].

Substituting the values of the parameters for O_2 into Eqs. (10), (12) at $V = J = 1$, we obtain the threshold of the energy quantum ΔT, the gain of which by the $O_2^-.(H_2O)_n$ system makes the latter stable: $\Delta T = 0.277$ eV.

Consequently, the maximum value is

$$T_{3G_g[O_2^-]} = T_{3G_g[O_2]} - \Delta T = 11.6866 \text{ eV} .$$

At the greater calculated values of the term $T_{3G_g[O_2^-]}$ only the $O_2^-.(H_2O)_n$ systems will exist in which the term of the p-state of O_2 corresponds to

$$T_{3G_u[O_2]} = 15.984 \text{ eV} .$$

We will determine the energy of binding of a water molecule with O_2^- in the cluster $O_2^-.(H_2O)_n$. The valence angle in H_2O for this cluster is 90.679^o and, according to [4], the parameter d is determined using scheme 2 presented in Fig. 1.

According to the data of [4], the O–K distance is 2.426 Å; then d (this is the H–K distance) is equal to 1.857 Å. Using formula (8) or (9), we find $T_{3G_g[O_2^-]}$; it turns out to equal 9.700 eV.

Substituting all the parameters into (1), we obtain the energy of binding of H_2O with O_2^-, which is equal to 0.818 eV. According to the data of [8], this quantity is 0.80 eV.

The term $T_{3G_g[O_2^-]}$ is determined by formula (9). Now knowing $T_{3G_g[O_2^-]}$, we pass to determination of the energy of binding of H_2O with O_2^- in the cluster $O_2^-.(H_2O)_n$ that is in "flint" water or in some other liquid products subjected to the flint action.

The value of a charge Δq is found as follows. In [9], we have shown that it is the charge passed on the water molecule adsorbed on flint causes the change in its valence angle. Consequently, in liquid "flint" water

$$\Delta q \text{ (liq } H_2O) = \Delta q \text{ (ad } H_2O) \, \Delta \alpha \text{ (liq } H_2O) / \Delta \alpha \text{ (ad } H_2O) . \tag{13}$$

For a mixture consisting mainly of water and ethyl alcohol it is necessary to find at first the portion of the charge transferred to one molecule of the adsorbed water and to one molecule of the adsorbed alcohol. The former is determined as

$$\Delta' q \,(ad\,H_2O) = \Delta' q \,(ad\,H_2O + ad\,CH_2CH_3OH) \,\Delta' \alpha \,(liq\,H_2O) \,[\Delta' \alpha \,(liq\,H_2O) + \Delta' \beta \,(liq\,CH_2CH_3OH)]^{-1} \,, \quad (14)$$

while the latter as

$$\Delta' q \,(ad\,CH_2CH_3OH) = \Delta' q \,(ad\,H_2O + ad\,CH_2CH_3OH) - \Delta' q \,(ad\,H_2O) \,. \quad (15)$$

The portion of the charge transferred by one molecule of water in the mixture filtered through flint is determined as

$$\Delta' q \,(liq\,H_2O) = \Delta q \,(ad\,H_2O) \,\Delta' \alpha \,(liq\,H_2O)/\Delta \alpha \,(ad\,H_2O) \,. \quad (16)$$

Results of the calculations of the energy of binding of H_2O with O_2 in the cluster $O_2^-.(H_2O)_n$ are presented in Table 1. In these calculations, the configuration of the cluster $O_2^-.(H_2O)_n$ for "flint" water is assumed to be similar to that of $O_2^-.(H_2O)_n$ for ordinary water. In blends, cognac spirits, cognacs, i.e., in systems that mainly consist of molecules of water and ethyl alcohol, the configuration of $O_2^-.(H_2O)_n$ corresponds to scheme 3 presented in Fig. 1.

From the calculations it follows that the energy of binding of one molecule of "flint" water in the cluster $O_2^-.(H_2O)_n$ with O_2^- is 16 times larger than the energy of binding of a molecule of ordinary water with an O_2 molecule and is equal to 12.642 kcal/mole.

The energy of this bond is close to:

(a) the energy of electron affinity in formation of a molecular negative oxygen ion (10–11.5 kcal/mole);

(b) the potential energy of vibration of a water molecule on its interaction with a negative molecular oxygen ion (12.5 kcal/mole);

(c) the energy of formation of a Bjerrum defect (11.9 kcal/mole) being a charge carrier from an adsorbed water molecule to an oxygen molecule.

In series of cognacs studied, the highest effect was obtained with the cognac prepared on "flint" cognac spirit (filtered once through flint), additionally the whole cognac was filtered once through columns filled with flint. For this variant of cognac, the binding energy was 0.4628 eV while the distance between the nuclei in the oxygen molecule (in the molecular ion) was equal to 1.2516 Å.

It should be noted that the distance between the nuclei in an oxygen molecule in "flint" water (presented in the table) is 1.236 Å; in the molecular oxygen dissolved in ordinary water it is 1.205 Å; in the negative ion of the molecular oxygen formed due to dissociative adhesion of electrons to a gas molecule at a high temperature the distance between the nuclei is 1.341 Å, and the lifetime of such an ion is $n \cdot 10^{-10}$ sec.

Thus, in the processes involved in filtration of liquids through flint, the state of molecular oxygen pertains to the intermediate one between O_2 and O_2^- and this state is stable in the environment of deformed molecules of water.

Now we pass to calculation of the energy of binding of a water molecule and of an ethyl-alcohol molecule with the negative ion of molecular oxygen. First we calculate the energy of binding of an ethyl alcohol with molecular oxygen. The scheme of interaction is shown in Fig. 2 (scheme 4).

To determine the binding energy, it is necessary to know the atomic terms $H_{(6)}$ and $C_{(2)}$ and the distances $H_{(6)}...K$ and $C_{(2)}...K$.

The atomic term of hydrogen $H_{(6)}$ in an ethyl-alcohol molecule is calculated as follows.

TABLE 1. Calculation of the Energy of Binding of the H_2O and CH_2CH_3OH Molecules with O_2 in Different Products

| Product	Water				Ethyl alcohol				Oxygen		Energy of binding with O_2, eV		
	$\Delta\alpha^0$	R, Å	d, Å	$T_{(H)}$, eV	$\Delta\beta_2^0$	R, Å	d, Å	$T_{(H)}$, eV	$T_{(O_2)}$, eV	$r' - r'_e$, Å	H_2O	CH_2CH_3OH	$H_2O + CH_2CH_3OH$
Softened water filtered once through flint ("flint" water)	+3.1	1.7430	1.8964	8.6526	–	–	–	–	11.4138	0.0308	0.5478	–	–
Blend prepared with "flint" water and "flint" spirit (the spirit is filtered once through flint)	+1.2	1.800	2.3927	8.8815	+1.8649	1.7593	2.3120	9.070	11.5301	0.0303	0.0423	0.0694	0.1117
Cognac prepared with the initial cognac spirit and additionally filtered once through flint	–2.3	1.8850	2.4817	9.8917	–1.6644	1.8424	2.4018	9.9014	11.3628	0.0388	0.4214	0.5581	0.9794
The same, two times filtered twice through flint	–2.2	1.8740	2.4670	9.5477	–1.5819	1.8316	2.3897	9.8802	11.3628	0.0374	0.2330	0.5566	0.7896
The same, filtered three times through flint	–1.5	1.8770	2.4665	9.4543	–0.8916	1.8345	2.3868	9.7065	11.5385	0.0234	0.1556	0.2979	0.4535
Cognac prepared with the "flint" cognac spirit and additionally filtered once through flint	–2.7	1.8980	2.4985	9.4381	–2.0555	1.8551	2.4186	10.003	11.1989	0.0466	0.6338	0.9636	1.5474
The same, filtered twice through flint	–0.2	1.8248	2.4048	9.1664	–0.138	1.7835	2.3224	9.1664	15.8940	0.0000	0.0057	0.0085	0.0142
The same, filtered three times through flint	–0.1	1.8250	2.4031	9.457	–0.229	1.7838	2.3225	9.5455	·15.8940	0.0000	0.0058	0.0091	0.0149
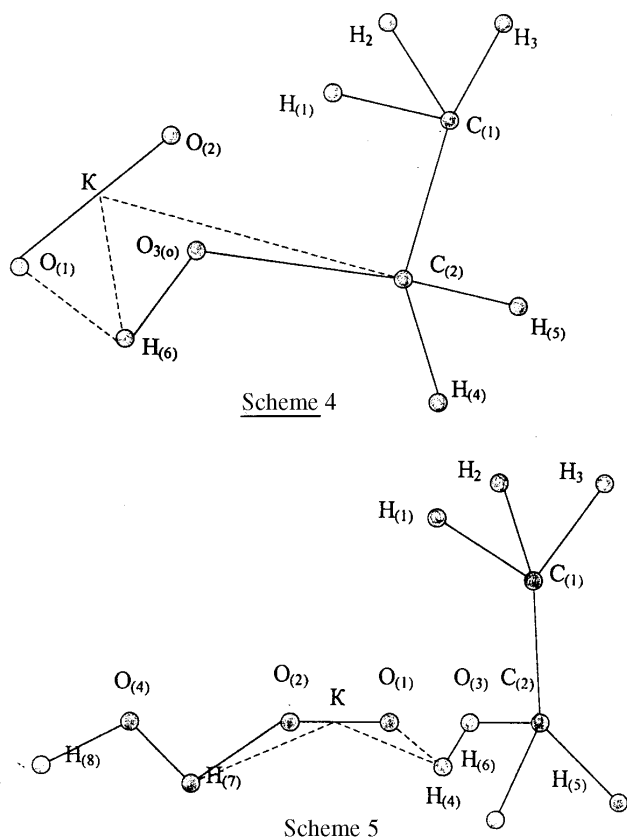
Fig. 2. Schemes of the interaction of the molecules of ethyl alcohol and
ethyl alcohol and water with molecular oxygen.

According to [10], the electron population of the atom in a molecule (the electron charge) and the order of bonds linearly depend on the force constants of bonds. The force constant of the O–H bond in the H_2O molecule is $12.8787 \cdot 10^6$ cm^{-2}; the force constant of the O–H bond in the CH_2CH_3OH molecule, according to the data [11], amounts to $12.6800 \cdot 10^6$ cm^{-2}.

The total electron charge on one hydrogen atom in an H_2O molecule is determined as 0.8225e [3]. Consequently, the term of the hydrogen atom in an ethyl-alcohol molecule is

$$T_{H(CH_2CH_3OH)} = (0.8225 \cdot 12.8787 / 12.6800)^2 \cdot 13.6 = 9.4911 \ eV.$$

The term of the oxygen atom $O_{(3)}$ of the p-state in an ethyl-alcohol molecule is determined as

$$T_{O(CH_2CH_3OH)} = (14.13 \cdot 3 + 9.4911)/4 = 12.9703 \ eV.$$

Now we determine the term of the hydrogen atom in the CH_2 and CH_3 groups of the ethyl-alcohol molecule.

According to [7], the electron population of hydrogen atoms in the CH_4, C_2H_4, and C_3H_8 molecules is 0.86e. Assuming a similar value for CH_2CH_3OH, we obtain

$$T_{H(CH_2CH_3OH)} = 0.86^2 \cdot 13.6 = 10.0585 \ eV.$$

The atomic term of carbon $C_{(1)}$ in the CH_3 group of the p-state is determined as a function of the terms of the p- and s-state of a free carbon atom and of the terms of the hydrogen atoms $H_{(1)}$, $H_{(2)}$, and $H_{(3)}$:

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$$T_{C(CH_3)} = 11.5795 \text{ eV} .$$

The atomic term of carbon $C_{(2)}$ of the p-state in the CH_2 group is determined as a function of the terms of the p- and s-state of a free carbon atom, of the atomic term of oxygen $O_{(3)}$ of the s-state, and of the atomic terms of hydrogen $H_{(3)}$ and $H_{(4)}$:

$$T_{C(CH_2)} = 13.1843 \text{ eV} .$$

Now we calculate the distance $H_{(6)}...K$. To do this, it is necessary to know the length of the hydrogen bond $H_{(6)}...O_{(1)}$.

According to [12], the distance between the neighboring atoms of oxygen $R_{(O-O)}$ in liquids, whose molecules are bound by hydrogen bridges, is determined as

$$\nu_{OH} = 3707 - 2.222 \cdot 10^7 \exp [- 3.925 R_{(O-O)}] . \tag{17}$$

As follows from [13], the vibration frequency of the O–H-group in a methyl-alcohol molecule (the number of vibrations 1, symmetry A') in a liquid is 3337 cm^{-1}, and for this mode of vibrations the position of a maximum of the band in the absorption spectrum of liquid water corresponds to a frequency of 3420 cm^{-1} [14]. Then for methyl and ethyl alcohols $R_{(O-O)}$ is equal to 2.8033 Å, and for water, to 2.8680 Å, i.e., the length of the hydrogen bond is

$$R_{(CH_2CH_3OH)} = R_{(H_2O)} R_{(O-O)(CH_2CH_3OH)} \big/ R_{(O-O)(H_2O)} . \tag{18}$$

The length of the donor-acceptor bond $H_{(6)}...K$ is 1.8828 Å, and the energy of this bond is 0.0465 eV. The length of the donor-acceptor bond $C_{(2)}...K$ is 3.6996 Å, and the energy of this bond is 0.6156 eV. The total energy of binding of an ethyl-alcohol molecule with molecular oxygen turns out to be 0.6621 eV, which is 19 times larger than the energy of binding of water with an oxygen molecule. It is this circumstance that is responsible for the higher solubility of oxygen in organic fluids with respect to water. According to the data of [15], oxygen has a 34-fold higher solubility in ethyl alcohol as compared with water.

Now we will calculate the energy of binding of one water molecule and one ethyl-alcohol molecule simultaneously with one oxygen molecule. A scheme of the interaction is presented in Fig. 2 (scheme 5).

In determining the term of the negative ion of oxygen, we account for the transfer of a charge to the oxygen molecules from the molecules of both water and ethyl alcohol.

The term of the hydrogen atom $H_{(6)}$ belonging to the O–H-group of the ethyl-alcohol molecule is determined in relation to the value of the valence angle $COH = \beta_2$ as follows:

$$T_{H\beta_2} = T_{H\beta_{2_{(0)}}} \left[\left(\frac{K_{\beta_2}}{K_{\beta_{2_{(0)}}}} - 1 \right) \frac{1}{2} + 1 \right]^2 , \quad T_{H\beta_{2_{(0)}}} = 9.4911 \text{ eV} . \tag{19}$$

In deriving formula (19), it has been taken into account that the change in the force constant of the valence angle causes the change in the electron population, in the order of the bonds $O_{(3)}-H_{(6)}$ and $H_{(3)}-C_{(2)}$ in the ethyl-alcohol molecule (i.e., it is distributed for three atoms).

According to [16],

$$\frac{K_{\beta_2}}{K_{\beta_{2_{(0)}}}} = \frac{[6 \sin^2 \beta_2 (1 - \cos \beta_2)^{-1} - 4 \cos \beta_2] [\sqrt{2 (1 - \cos \beta_{2_{(0)}})^3}]}{[6 \sin^2 \beta_{2_{(0)}} (1 - \cos \beta_{2_{(0)}})^{-1} - 4 \cos \beta_{2_{(0)}}] [\sqrt{2 (1 - \cos \beta_2)^3}]} . \tag{20}$$

Calculated results of the energy of binding of one water molecule and one ethyl-alcohol molecule with one oxygen molecule (the negative ion of oxygen) are given in Table 1.

As follows from the table, in all cases the energy of binding of the ethyl-alcohol molecule with the oxygen molecule is higher than the energy of binding of the water molecule with the same oxygen molecule. The highest binding energy is observed in the case of cognac prepared with "flint" cognac spirit and with cognac additionally filtered once through flint.

From the results presented it also follows that the energy of binding of a water molecule and an ethyl-alcohol molecule with molecular oxygen directly depends on the amount of active oxygen (the negative ions of molecular oxygen) in a liquid.

The accumulation of active oxygen causes a change in the palatability and in the bouquet of a number of foodstuffs.

NOTATION

ε_s^c, atomic term of the anion of the s-state; ε_p^a, atomic term of the anion of the p-state; $T_{3G_g[O_2^-]}$, term of the electrons of the p-state of the orbital $3G_u$ of the molecular ion O_2^-; $T_{3G_g[O_2]}$, term of the electrons of the p-state of the orbital $3G_u$ of the O_2 molecule; $D_{0[O_2^-]}$, dissociation energy of O_2^-; $D_{0[O_2]}$, dissociation energy of O_2; r_e', equilibrium distance between the nuclei in the O_2 molecule; r', equilibrium distance between nuclei in O_2^-; Δq, relative value of the transferred charge; T, T_e, $G_{(V)}$, and $F_{V(J)}$, total, electronic, vibrational, and rotational energy of a molecule, respectively; V, vibrational quantum number; J, rotational quantum number; $X_e\omega_e$, anharmonism constant; B_e, rotational constant; a_e, binding constant; $\Delta q(\text{liq H}_2\text{O})$ and $\Delta\alpha(\text{liq H}_2\text{O})$, charge and the change in the valence angle in liquid "flint" water; $\Delta' q(\text{ad H}_2\text{O})$ and $\Delta\alpha(\text{ad H}_2\text{O})$, charge and the change in the valence angle in water molecule adsorbed on flint; $\Delta' q(\text{ad H}_2\text{O} + \text{ad CH}_2\text{CH}_3\text{OH})$, total charge transferred to one adsorbed water molecule and to one adsorbed ethyl-alcohol molecule (calculated from the data on deformation of the flint lattice under conditions of mixture adsorption); $\Delta'\alpha(\text{liq H}_2\text{O})$, change in the valence angle in the molecule of water in the blend (the mixture of water and ethyl alcohol); $\Delta'\beta(\text{liq CH}_2\text{CH}_3\text{OH})$, change in the sum of valence angles in the ethyl-alcohol molecule; $T_{\text{H(CH}_2\text{CH}_3\text{OH)}}$, term of the hydrogen atom in the ethyl-alcohol molecule; $T_{\text{O(CH}_2\text{CH}_3\text{OH)}}$, term of the oxygen atom $O_{(3)}$ of the p-state in the ethyl-alcohol molecule; $T_{\text{C(CH}_3)}$ and $T_{\text{C(CH}_2)}$, terms of the carbon atoms in the CH_3 and CH_2 groups of the ethyl-alcohol molecule; ν_{OH}, frequency of stretching vibrations in the O–H group in liquids; $K_{\beta_{2_{(0)}}}$, force constant of the valence angle $C_{(2)}O_{(3)}H_{(6)}$ at a value of 108.9°; $K_{\beta_{2_{(2)}}}$, force constant of the valence angle $C_{(2)}O_{(3)}H_{(6)}$ at any other value of it; K, coordinate of the center between the nuclei in the oxygen molecule.

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